

# MACROMOLECULAR POWDER DIFFRACTION: STRUCTURE SOLUTION VIA MOLECULAR REPLACEMENT

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## INTRODUCTION

Macromolecular powder diffraction is a burgeoning technique for protein structure solution— ideally suited for cases where no suitable single crystals are available. Over the past seven years, pioneering work by Von Dreele *et al.* (1) and Margiolaki *et al.* (2), demonstrated the viability of this approach for several protein structures. Among these initial powder studies, molecular replacement solutions of insulin and turkey lysozyme into alternate space groups were accomplished. Pressing the technique further, Margiolaki, *et al.* (3), executed the first molecular replacement of an unknown protein structure: the SH3 domain of ponsin.

## RESULTS

To demonstrate that cross-species molecular replacement is also possible, we present the solution of hen egg white lysozyme using the 60% identical human lysozyme (PDB code: 1LZ1) as the search model (see Figure 1). Due to the high incidence of overlaps in powder patterns, especially as structures get more complex, we have used extracted intensities from five data sets taken at different salt concentrations in a multi-pattern Pawley refinement.

## REFERENCES

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3. I. Margiolaki, I., J.P. Wright, M. Wilmanns, A.N. Fitch, and N. Pinotsis *J. Am. Chem. Soc.*, 129, 11865 (2007).

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Figure 1: Superposition of the PSSP trial two result (black) and the previously published HEWL structure (grey).